

# Simulations of Two-Dimensional Unbiased Polymer Translocation Using the Bond Fluctuation Model

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## Abstract

We use the Bond Fluctuation Model (BFM) to study the pore-blockade times of a translocating polymer of length  $N$  in two dimensions, in the absence of external forces on the polymer (i.e., unbiased translocation) and hydrodynamic interactions (i.e., the polymer is a Rouse polymer), through a narrow pore. Earlier studies using the BFM concluded that the pore-blockade time scales with polymer length as  $\tau_d \sim N^\beta$ , with  $\beta = 1 + 2\nu$ , whereas some recent studies with different polymer models produce results consistent with  $\beta = 2 + \nu$ , originally predicted by us. Here  $\nu$  is the Flory exponent of the polymer;  $\nu = 0.75$  in 2D. In this paper we show that for the BFM if the simulations are extended to longer polymers, the purported scaling  $\tau_d \sim N^{1+2\nu}$  ceases to hold. We characterize the finite-size effects, and study the mobility of individual monomers in the BFM. In particular, we find that in the BFM, in the vicinity of the pore the individual monomeric mobilities are heavily suppressed in the direction perpendicular to the membrane. After a modification of the BFM which counters this suppression (but possibly introduces other artifacts in the dynamics), the apparent exponent  $\beta$  increases significantly. Our conclusion is that BFM simulations do not rule out our theoretical prediction for unbiased translocation, namely  $\beta = 2 + \nu$ .

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## I. INTRODUCTION

For polymer translocation through narrow pores in membranes, the scaling behavior of pore-blockade times with the length of linear polymers has been a topic of intense research in recent times. Such interest in polymer translocation has been fueled by its obvious biological context; i.e., molecular transport through cell membranes, which is an essential mechanism in living organisms. Often, the molecules are too long, and the pores in the membranes too narrow, to allow the molecules to pass through as a single collapsed unit. In such circumstances, the molecules have to deform themselves in order to squeeze — i.e., translocate — through the pores. Parallelly, the urge to understand the dynamics of translocation also stems from the fact that new developments in design and fabrication of nanometer-sized pores and etching methods, in recent times, have put translocation at the forefront of single-molecule experiments, with the hope that translocation may lead to cheaper and faster technology for the analysis of biomolecules.

Although significant progress has been made in the last few years in the field of both theory and simulations of polymer translocation, consensus among different research groups on the scaling behavior of the characteristic time  $\tau_d$  that the polymer spends in the pore, with the length  $N$  of a linear polymer, characterized by an exponent  $\beta \equiv \partial(\log(\tau_d))/\partial(\log(N))$ , has generally remained elusive. Of the three main translocation situations studied theoretically or by computer simulations, namely (i) unbiased translocation, wherein the polymer translocates purely due to thermal fluctuations, (ii) field-driven translocation, wherein translocation is driven by a potential difference across the pore, and (iii) pulled translocation, wherein translocation is facilitated by a pulling force at the head of the polymer, unbiased translocation is by far the most fiercely debated topic.

From a statistical physics perspective, the translocation problem can be seen as a kind of a tunneling process over an entropic barrier. This entropic barrier arises because the number of states available to the polymer is significantly decreased by the presence of the membrane. For a polymer of length  $N$ , the number of states in the bulk scales as  $Z_b(N) \approx A \mu^N N^{\gamma-1}$  in which  $\gamma$  is a universal exponent —  $\gamma = 49/32$  and  $\gamma \approx 1.16$  in two and three dimensions, respectively — while  $A$  and  $\mu$  are not universal. The corresponding number of states for the same polymer, but whose end is tethered to the membrane, is approximated by  $Z_w(N) \approx A_1 \mu^N N^{\gamma_1-1}$  in which the parameter  $\mu$  is not affected by the introduction

of the membrane,  $\gamma_1$  is a different universal exponent —  $\gamma_1 = 61/64$  and  $\gamma_1 \approx 0.68$  in two and three dimensions, respectively — while  $A_1$  is again not universal. Consider the translocating polymer, for which there are  $n$  monomers on one side and  $(N - n)$  monomers on the other. Since this situation can be seen as two strands of polymers with one end (of each strand) tethered on the membrane, the number of states for this polymer is given by  $Z_w(n)Z_w(N - n)$ , which attains a minimum when  $n = N/2$ . The effective entropic barrier faced by a translocating polymer is thus

$$\Delta S = \log \left( \frac{Z_b(N)}{Z_w(N/2)^2} \right) = c \log(N) + k, \quad (1)$$

with  $c = \gamma - 2\gamma_1 + 1$  and  $k = \log(A) - 2 \log(A_1) + 2(\gamma_1 - 1) \log(2)$ .

In 2001, Chuang *et al.* [1] established that the then existing mean-field type descriptions based on the Fokker-Planck equation for first-passage over this entropic barrier [2–4] are unsuitable for describing unbiased translocation. In the absence of explicit hydrodynamics, i.e., for a Rouse polymer, Chuang *et al.* [1] argued that the pore-blockade time (or the dwell time)  $\tau_d$  cannot be less than the the Rouse time, which scales as  $\tau_R \sim N^{1+2\nu}$ . Based on simulations in 2D using the BFM, with  $N = 128$  or less, they further concluded that the ratio of the dwell and Rouse times is approximately constant, suggesting that  $\beta = 1 + 2\nu$  as well. As it later turned out, the paper by Chuang *et al.* initiated a flurry of theoretical and simulation works on unbiased translocation.

For a number of years following the work by Chuang *et al.* [1], several simulation studies reported the exponent for the pore-blockade time for unbiased translocation both in 2D and 3D to be consistent with  $1 + 2\nu$  (which in 2D equals 2.5, and  $\approx 2.18$  in 3D) for a Rouse polymer [5–7]. Some of these studies characterized the anomalous dynamics of unbiased translocation as well: having denoted the monomer number at the pore by  $s(t)$  at time  $t$ , the mean-square displacement of the monomers  $\langle \Delta s^2(t) \rangle$  through the pore in time  $t$  was found to scale  $\sim t^\alpha$  with  $\alpha = 2/(1+2\nu)$ , satisfying the obvious requirement  $\langle \Delta s^2(\tau_d) \rangle = N^2$ . Over the last couple of years however, several other studies on unbiased translocation have been performed for a Rouse polymer, whose scaling results for  $\beta$  and  $\alpha$  differ from  $1 + 2\nu$  and  $2/(1 + 2\nu)$  respectively. In 2007 and 2008, using a theoretical approach based on polymer's memory effects, aided by simulations with a highly efficient lattice polymer model (developed by ourselves) we showed that for a Rouse polymer  $\langle \Delta s^2(t) \rangle \sim t^{(1+\nu)/(1+2\nu)}$  [i.e.,  $\alpha = (1+\nu)/(1+2\nu)$ ] up to the Rouse time  $\tau_R$ , and thereafter  $\langle \Delta s^2(t) \rangle \sim t$  [i.e.,  $\alpha = 1$ ] as no

Authors	$\beta$ (2D, Rouse)	$\beta$ (2D, Zimm)	$\beta$ (3D, Rouse)	$\beta$ (3D, Zimm)
Chuang <i>et al.</i> [1]	$1 + 2\nu = 2.5$ (BFM)	—	—	—
Luo <i>et al.</i> [5]	$2.50 \pm 0.01$ (BFM)	—	—	—
Huopaniemi <i>et al.</i> [6]	$2.48 \pm 0.07$ (FENE MD)	—	—	—
Wei <i>et al.</i> [7]	$2.51 \pm 0.03$ (bead-spring MD)	—	2.2 (bead-spring MD)	—
Chatelain <i>et al.</i> [16]	2.5 (BFM)	—	—	—
Luo <i>et al.</i> [17]	$2.44 \pm 0.03$ (GROMACS)	— —	$2.22 \pm 0.06$ (GROMACS)	— —
Panja <i>et al.</i> [8, 9]	—	—	$2 + \nu \approx 2.588$	$1 + 2\nu \approx 2.18$
Panja <i>et al.</i> [10]	$2 + \nu = 2.75$	$1 + 2\nu = 2.5$	—	—
Dubbeldam <i>et al.</i> [12]	—	—	$2.52 \pm 0.04$ (FENE)	—
Gauthier <i>et al.</i> [13]	—	—	$2 + \nu$	$1 + 2\nu$
Guillouzic <i>et al.</i> [14]	—	—	—	2.27 (MD)
Gauthier <i>et al.</i> [15]	—	—	—	11/5=2.2 (MD)

TABLE I. Summary of all the results on the exponent for the pore-blockade time for unbiased translocation known to us at the time of writing this paper. Abbreviations used: MD (molecular dynamics), FENE (Finite Extension Nonlinear Elastic).

memory in the polymer survive beyond the Rouse time; consequently, the exponent for the pore-blockade time is given by  $\beta = 2 + \nu$ , i.e.,  $\approx 2.588$  in 3D [8, 9] and 2.75 in 2D [10]. In the presence of hydrodynamics, i.e., for a Zimm polymer,  $\langle \Delta s^2(t) \rangle$  was predicted to behave  $\sim t^{(1+\nu)/(3\nu)}$  up to the Zimm time  $\tau_Z \sim N^{3\nu}$ , and thereafter  $\langle \Delta s^2(t) \rangle \sim t$ ; leading to the expectation that  $\tau_d$  should scale as  $N^{1+2\nu}$  [8, 9]. (We showed that the fact that  $\beta = 1 + 2\nu$  for a Zimm polymer has nothing to do with Rouse dynamics. It is in fact a pure coincidence that this exponent is the same as the Rouse exponent, as explained in Ref. [8, 9]). We showed that these memory effects stem from the polymer's local strain relaxation in the neighborhood of the pore [8–11].

Recent numerical results, using completely different polymer models from ours, obtained by Dubbeldam *et al.* [12], and by Gauthier and Slater [13] agree very well with  $\beta = 2 + \nu$  for a Rouse polymer. For a Zimm polymer, Gauthier and Slater [13], and further works by Guillouzic and Slater [14], and by Gauthier and Slater [15] reported  $\beta = 1 + 2\nu$ ; these are consistent with our scaling prediction [8, 9], but we note that Ref. [13] reports this result using an approach which differs from ours. Thus, while the two contenders for  $\beta$  have emerged to be (a)  $1 + 2\nu$  for a Rouse polymer, originally proposed by Chuang *et al.* [1], and (b)  $2 + \nu$  for a Rouse, and  $1 + 2\nu$  for a Zimm polymer, originally predicted by us [8–10], the publication of two recent papers [5, 16] that reassert their authors' earlier result  $\beta = 1 + 2\nu$  for unbiased translocation for a Rouse polymer indicates that the debate is not yet settled.

Before proceeding further, for the benefit of the readers, in Table I we summarize all the results on the exponent for the pore-blockade time for unbiased translocation known to us to date.

Given that our theoretical arguments for  $\beta = 2 + \nu$  for unbiased translocation of Rouse polymers are seemingly at odds with a number of simulations, reporting exponents much closer to  $\beta = 1 + 2\nu$ , we decided to redo the latter simulations. It is impossible for us to analyze in detail each and every model that has been used to produce  $\beta = 1 + 2\nu$  for a Rouse polymer; nevertheless, having seen that the BFM has been frequently used to obtain this result, we prompt ourselves to revisit unbiased translocation in 2D for a Rouse polymer, using *exactly the same details* of the BFM used by Chuang *et al.* [1].

First, we extend the range of polymer lengths studied, from  $N \leq 256$  [1, 5, 16] up to  $N = 1000$ . While the reported behavior for  $N \leq 256$  [1, 5, 16] is that the function  $f(N) \equiv \tau_d/N^{1+2\nu}$  is constant within numerical accuracy, our simulations with longer polymers reveal  $f(N)$  to be a monotonically decreasing quantity with increasing  $N$ , with a rate of decrease for  $f(N)$  which increases with increasing  $N$ . The conclusion is that the reported constant behavior of  $f(N)$  corresponds to an *effective* exponent of  $\beta \approx 1 + 2\nu$ , which does not hold for long polymers.

Secondly, for the BFM, having established the above for  $\tau_d$ , we set out to quantify the finite-size effects in various basic equilibrium quantities that play a role in the dynamics of translocation. These are (i) the equilibrium end-to-end distance, (ii) the (equilibrium) entropic spring constant, and (iii) the longest correlation time for a tethered polymer at equilibrium as a function of their length. We find, for the BFM, that the finite-size effects

for (i) are negligible (data not shown in this paper), but the finite-size effects for (ii) and (iii) are severe. Once these finite-size effects are taken into account, the polymer's memory effects for the BFM do not rule out those we found in Refs. [8, 9], which originally reported  $\beta = 2 + \nu$ .

Thirdly, and quite remarkably, these finite-size effects still do not explain the peculiar behaviour of  $f(N)$  for the BFM. We therefore also study a dynamic quantity, namely the mobility of individual monomers in the BFM, as a function of monomer number and direction. Especially for the monomers in the vicinity of the pore, this dynamic quantity shows highly anomalous behavior. We find that when this behavior is corrected towards how one expects the monomers to behave in the neighborhood of the pore, the exponent for the pore-blockade time increases towards  $2 + \nu$ . We therefore conclude that the BFM is a fine model for polymer dynamics in general, but does not handle situations very well where the polymer is constrained to pass through a narrow pore. Our analysis also implies that for those polymer models that assert  $\beta = 1 + 2\nu$ , one needs to thoroughly investigate their finite-size effects and dynamical peculiarities, if such an assertion is to prove meaningful.

The organization of this paper as follows. In Sec. II we briefly discuss the BFM, and the details of the used BFM variant in this paper. In Sec. III we study finite-size effects in the BFM for several equilibrium properties. In Sec. IV we study with the BFM the quantity  $f(N) = \tau_d/N^{1+2\nu}$ , and find that it is a monotonically decreasing quantity with increasing  $N$ , such that the rate of decrease for  $f(N)$  increases with increasing  $N$ ; this result implies that the reported exponent  $\beta = 1 + 2\nu$  for Rouse polymers is an *effective* exponent which does not hold in the limit  $N \rightarrow \infty$ , contrary to the conclusions of Refs. [1, 5, 16, 17]. In Sec. IV we also show that we do not find  $\alpha = 2/(1 + 2\nu)$  [= 0.8 in 2D], while we do find a diffusive regime for the anomalous dynamics of translocation, contradicting the claims of Ref. [5]. In Sec. IV A we demonstrate that once the finite-size effects in various basic quantities for the BFM are taken into account, the polymer's memory effects for the BFM are entirely consistent with those we found in Refs. [8, 9], which originally reported  $\beta = 2 + \nu$ . In Sec. VI we trace the peculiarities of the BFM to the anomalous behavior of the mobility of individual monomers in the neighborhood of the pore. We conclude the paper in Sec. VII.

All throughout this paper, following the convention of the existing literature, we denote the monomer number located in the pore at time  $t$  by  $s(t)$ .

## II. THE BOND FLUCTUATION MODEL (BFM)

The two-dimensional bond fluctuation model, introduced by Carmesin and Kremer in 1988 [18], is a very frequently used model for the simulation of polymer dynamics. In the original form of the model, each monomer occupies four ( $2 \times 2$ ) lattice sites of a square lattice: thus two monomers are always separated by at least a distance of two lattice spacings. Monomers adjacent in the polymer are connected by bonds with lengths between 2 and  $\sqrt{13}$ . The original model is illustrated for a polymer through a membrane of thickness two lattice sites in Fig. 1, with monomer 4 residing within the pore that is three lattice sites wide.

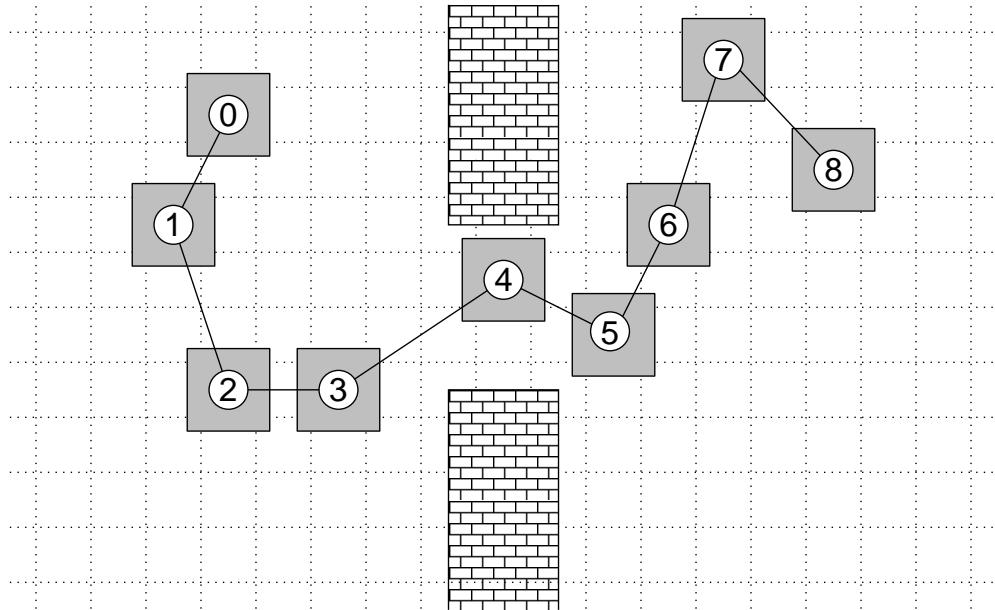


FIG. 1. The original bond fluctuation model in 2D, due to Carmesin and Kremer [18], illustrated for a polymer translocating through a membrane thickness of two lattice sites thickness, with monomer 4 residing within the pore that is three lattice sites wide. Monomers reside on a square lattice. Adjacent monomers are connected by a bond, which can only take lengths of 2,  $\sqrt{5}$ ,  $2\sqrt{2}$ , 3,  $\sqrt{10}$ , or  $\sqrt{13}$ . The excluded area around each monomer consists of  $2 \times 2$  lattice sites. The particular choice for the values allowed to the bond length, in combination with the size of the excluded area, suffices to avoid the crossing of bonds. In simulations of translocation, the membrane is represented as a line with a thickness of 2 sites, with a pore of 3 lattice sites wide. The dynamics of the polymer consists of single-monomer hops to nearest-neighbor lattice sites, restricted by the constraints on bond length and excluded volume.

As mentioned already, in this paper we use exactly the same model as that of Ref. [1], which is a variation on the original BFM due to Carmesin and Kremer. Its details are as follows. Hydrodynamic interactions are not considered in this model. The  $N$  monomers of the polymer reside on a square lattice. Excluded volume interactions are implemented by forbidding two monomers to be closer than 2 lattice units, while the sequential connectivity of the monomers are maintained by requiring the separation between the adjacent monomers of the polymer to be less than or equal to  $\sqrt{10}$  lattice units. This choice of the minimal and the maximal distances ensures that the polymer never intersects itself. The dynamics of the model is implemented by Monte Carlo moves: An elementary move consists of an attempt to move a randomly selected monomer by one lattice spacing in an arbitrarily chosen direction. If the new configuration is permitted, the move is accepted; otherwise, the move is rejected. The unit of time in this model is defined by  $N$  attempted MC moves for the entire polymer. We choose a box size of  $10N \times 10N$ ; and the membrane, with a thickness of two lattice units, divides the box into two equal chambers of size  $10N \times 5N$ , with the pore of width three lattice units exactly at the center of the box. The tight size of the pore ensures that the monomer  $s$  residing within the pore is uniquely defined at any time. For each realization, we first tether the polymer halfway at the pore, with  $N/2$  monomers on each side of the membrane, and equilibrate it for times typically  $> 100N^{1+2\nu}$ . We then remove the tether at time  $t = 0$  and wait till the polymer disengages from the pore. The averages are obtained over an ensemble of such realizations: we use 16,384 realizations for  $N < 1000$  and 2,048 realizations for  $N = 1000$ . We define the mean time  $\tau_u$  that the polymer takes to disengage from the pore to either side of the membrane as the characteristic unthreading time for the polymer. For unbiased translocation, the scaling of the unthreading time with polymer length is the same as that of  $\tau_d$  [9].

### III. EQUILIBRIUM PROPERTIES FOR THE BFM

Two main ingredients for the derivation of  $\beta = 2 + \nu$  for a Rouse polymer, as predicted by us [8–10], are the following well-known properties of Rouse polymers. For a polymer of length  $N$  with one end tethered on a membrane, (i) the inverse entropic spring constant should scale as  $N^{2\nu}$  [19], and (ii) the equilibrium correlation function for the tether-to-end vector must scale as  $N^{1+2\nu}$ . We now check for both properties.

$N$	$\langle R_e \rangle$	$\langle R_e^2 \rangle$	$\mathcal{R}^2$	$\mathcal{R}^2/(N/2)^{2\nu}$
20	13.60	197.8	12.90	0.408
30	18.39	363.7	25.40	0.437
40	22.81	560.9	40.74	0.455
50	26.92	783.2	58.66	0.469
60	30.83	1029.5	78.83	0.480
80	38.20	1583.7	124.5	0.492
100	45.13	2213.5	176.9	0.500
150	61.01	4056.3	334.5	0.515
200	75.67	6247.0	520.3	0.520
300	102.4	11455	969.4	0.528
500	149.9	24584	2108	0.533
700	193.0	40751	3513	0.537
1000	252.2	69616	6018	0.538

TABLE II. Scaling of the inverse entropic spring constant  $\mathcal{R}^2$  of the polymer, data averaged over  $10^7$  realizations, which are separated by one pivot move and  $N$  BFM moves; this corresponds roughly to a million statistically independent measurements. The systematic trend as shown in 5th column demonstrates the strong finite-size effects in the BFM.

### A. Entropic spring constant of the polymer

With the polymer threaded halfway at the pore, i.e., effectively for a polymer of length  $N/2$  with one end tethered on the membrane, we denote the distance of the free ends of the polymer from the pore by  $R_e$ , and then the inverse of the spring constant of the polymer is  $\propto \mathcal{R}^2 = \langle R_e^2 \rangle - \langle R_e \rangle^2$  [19], where the angular brackets denote the average over the equilibrium ensemble — equilibrium is achieved by applying a million pivot moves to each realization upon tethering one end of the polymer on the membrane. For long polymers the inverse entropic spring constant  $\mathcal{R}^2$  should scale as  $N^{2\nu}$ . Since this quantity is an equilibrium property, we combined the usual single-monomer moves of the BFM with pivot moves, in which rotations of the polymer tails by  $\pm 90$  degrees around a randomly selected monomer

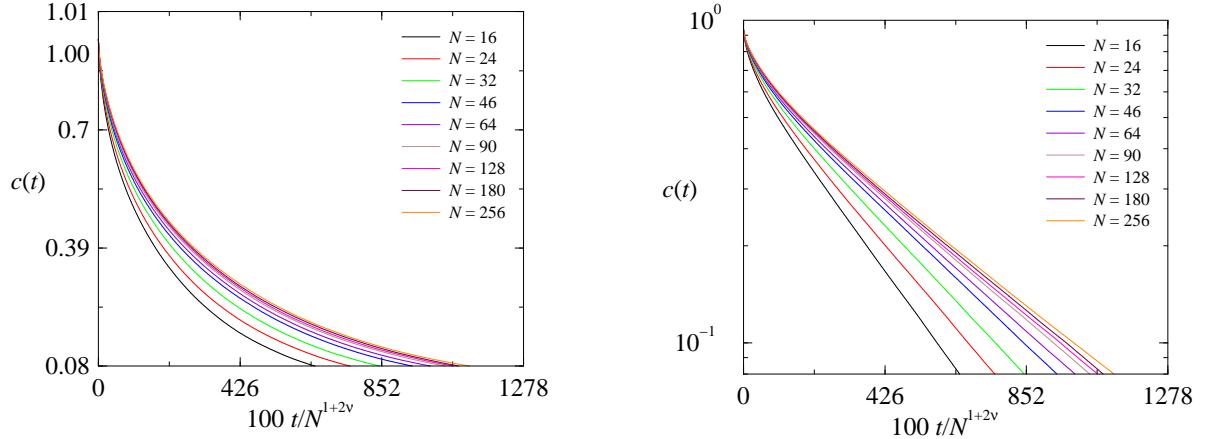


FIG. 2. Plot of the correlation function  $c(t)$  for different values of  $N$ : linear scale (left panel), semi-log scale (right panel), with  $\nu = 0.75$  in 2D. The lack of collapse demonstrates the presence of strong finite-size effects in the dynamical properties of polymers in BFM. The  $N = 256$  data corresponds well to  $c_{(N=256)}(t) \sim \exp[-t/(5.8 \times 10^6)]$ . Data averaged over 16,384 independent realizations.

are attempted, and accepted if the resulting configuration is valid. With pivot moves, care has to be taken that not only overlapping monomers cause rejection: also attempted moves to other configurations which are not accessible via a sequence of the usual single-monomer moves should be rejected. Because of the fast decorrelation of the combined algorithm, accurate measurements could be obtained. The finite-size effects in the scaling of  $\mathcal{R}^2$  are shown in Table II.

### B. Equilibrium correlation function for the tether-to-end vector for the BFM

Similarly, for a polymer of length  $N/2$  with one end tethered on the membrane, we denote the vector distance of the free end of the polymer w.r.t. the tethered end at time  $t$  by  $\mathbf{e}(t)$ , and define the correlation function for the tether-to-end vector as

$$c(t) = \frac{\langle \mathbf{e}(t) \cdot \mathbf{e}(0) \rangle - \langle \mathbf{e}(t) \rangle \cdot \langle \mathbf{e}(0) \rangle}{\sqrt{\langle \mathbf{e}^2(t) - \langle \mathbf{e}(t) \rangle^2 \rangle \langle \mathbf{e}^2(0) - \langle \mathbf{e}(0) \rangle^2 \rangle}}. \quad (2)$$

The angular brackets in Eq. (2) denote averaging in equilibrium. Here equilibrium means that with one end tethered on the membrane the polymer is thermalized for times  $> 100N^{1+2\nu}$ . The quantity  $c(t)$  is plotted in Fig. 2 for several values of  $N \leq 256$ , in lin-

ear as well as in semi-log plots. The lack of collapse in Fig. 2, together with the data of Table I, demonstrates that the finite-size effects in this model are severe.

## IV. ASYMPTOTIC SCALING OF $\tau_d$ , AND ANOMALOUS DYNAMICS OF UNBIASED TRANSLOCATION IN THE BFM

### A. In the BFM the scaling $\tau_d \sim N^{1+2\nu}$ does not hold asymptotically

Having shown that the finite-size effects of the BFM are significant at least up to lengths of a few hundred monomers, below in Table III we present the results of the mean unthreading time  $\tau_u$  over a wide range of values of  $N$ . From Table III we find that for the BFM the quantity  $f(N) = \tau_d/N^{1+2\nu}$  is a monotonically decreasing quantity with increasing  $N$ , such that the rate of decrease for  $f(N)$  increases with increasing  $N$ . Having noted that for the BFM, the conclusion that  $\beta = 1 + 2\nu$  has been based on simulation data for  $N \leq 256$  [1, 5, 16, 17], the finite-size effects in this model as demonstrated in Sec. III and the data of Table III imply that there is no convincing numerical evidence that the exponent  $\beta$  approaches the value  $1 + 2\nu$  in the thermodynamic limit ( $N \rightarrow \infty$ ), contrary to the conclusions of Refs. [1, 5, 16, 17]. Rather, it is an *effective* exponent, approximately valid over a finite range of polymer lengths. It is worthwhile to mention here that in contrast to the behavior of  $\beta$  obtained from the BFM, our result  $\beta = 2 + \nu$  for a Rouse polymer has been checked for  $N$  up to 500 [8, 9], and up to 1000 [20] in our lattice polymer model, and we have shown that in our model the finite-size effects become undetectable beyond  $N = 150$  [9].

### B. Anomalous dynamics of unbiased translocation in the BFM

Next we focus on the anomalous dynamics of unbiased translocation in the BFM. The standard way to study the anomalous dynamics is to plot  $\langle \Delta s^2(t) \rangle$  as a function of  $t$ , as discussed in the introduction; however, it comes with the following disadvantage. With the initial condition  $s(t = 0) = N/2$ ,  $\Delta s$  is undefined once the polymer disengages from the pore, and as a result,  $\langle \Delta s^2(t) \rangle$  saturates in time fairly quickly [16]. To avoid such saturation effects, we study the anomalous dynamics of translocation in a somewhat non-standard

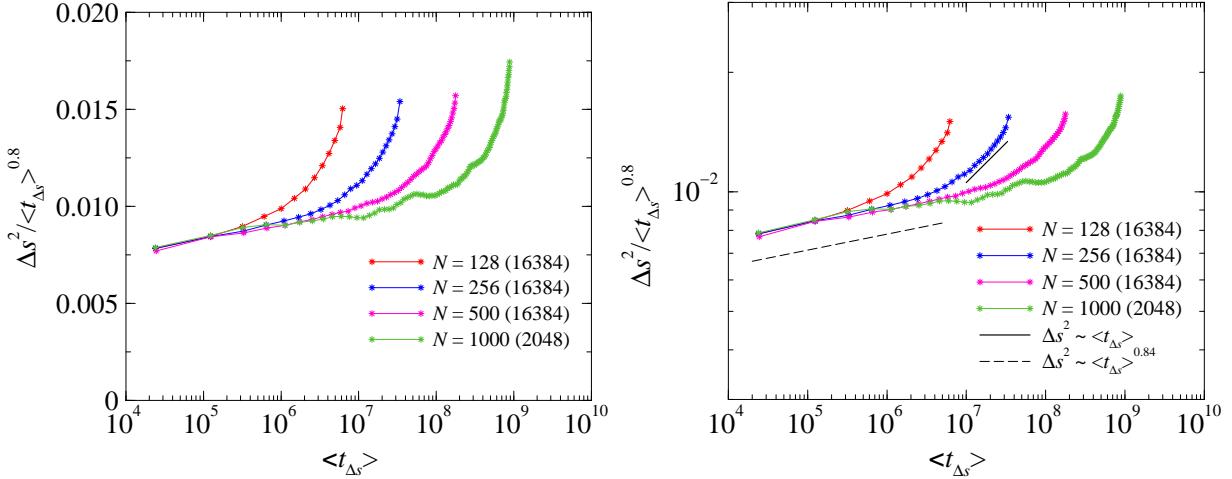


FIG. 3. Plots of  $\Delta s^2/\langle t_{\Delta s} \rangle^{0.8}$  as a function of  $\langle t_{\Delta s} \rangle$  with  $|\Delta s| = 5, 10, 15, \dots, N/2$ : semi-log (left panel), log-log (right panel). The numbers in the parentheses in the legends denote the number of independent realizations over which the averages have been calculated. If indeed  $\langle \Delta s^2(t) \rangle$  were to scale as  $t^{2/(1+2\nu)} = t^{0.8}$ , both panels would have produced horizontal lines. The lowest exponent  $\alpha$  for  $\langle \Delta s^2(t) \rangle \sim t^\alpha$  obtained for each curve is 0.84, which gradually crosses over to diffusive regime (for  $|\Delta s|$  close to  $N/2$ , because of entropic reasons,  $\alpha > 1$ ); at a contrast to this,  $\alpha = 0.86$  has been reported in Ref. [16] all throughout; implying that the value of  $\alpha$  reported in Ref. [16] is an effective value. Additionally there is a diffusive regime, contrary to the claims of Ref. [17], as shown by the solid black line in the right panel. As explained in the text, this diffusive regime is to be expected since the mean unthreading time is much longer than the longest relaxation times of the polymers. The plots are clearly consistent with the data in Table II, namely that the coefficient  $\tau_u/N^{1+2\nu}$  is a decreasing function of  $N$ .

form. We calculate the mean first passage time  $\langle t_{\Delta s} \rangle$  of arrival at a monomeric distance  $\Delta s \equiv |s(t) - N/2|$ . Thus, in each simulation, starting with  $s = N/2$  at  $t = 0$ , we keep track of the first arrival times  $t_{\Delta s}$  for all values of  $\Delta s = 1 \dots N/2$ . In this manner, at no point in time the data suffer from saturation problems. The idea behind obtaining  $t_{\Delta s}$  as a function of  $\Delta s$  is actually motivated by the observation that  $\tau_u$  is the mean first passage time for  $\Delta s = N/2$ .

To verify whether the purported scaling  $\langle \Delta s^2(t) \rangle \sim t^\alpha$  with  $\alpha = 2/(1+2\nu)$  [1, 5, 16] holds, we plot  $\Delta s^2/\langle t_{\Delta s} \rangle^{0.8}$  in Fig. 3 as a function of  $\langle t_{\Delta s} \rangle$  (left panel: log-linear, right panel: log-log). The data should then be constant so long as the polymer remains threaded

within the pore, since  $1 + 2\nu = 0.8$  in 2D. However, as Fig. 3 demonstrates, we do not find any evidence for  $\alpha = 2/(1+2\nu) = 0.8$ ; the lowest value of  $\alpha$  we find is 0.84 (dashed line in the right panel of Fig. 3), which slowly crosses over to diffusive behavior at long times [contrary to the report of Ref. [5], where, based on  $\langle \Delta s^2(t) \rangle$  data till  $t \lesssim 10^3$ , it has been concluded that there is no diffusive regime for the dynamics of unbiased translocation]. In this context, note that close to  $|\Delta s| = N/2$ , the effective exponent  $\alpha$  exceeds 1, as it should be, since close to the end, an entropic driving force takes over, giving rise to a non-negligible velocity of translocation. The diffusive behavior is illustrated in the right panel of Fig. 3 for  $N = 256$ ; the existence of the diffusive regime is expected to show beyond the autocorrelation time, which for a polymer of length  $N = 256$  equals  $\tau_c \approx 5.8 \times 10^6$  (see Fig. 2), but well below the unthreading time  $\tau_u^{(N=256)} \approx 3.8 \times 10^7$ . Also note here that  $\alpha > 0.8$  is consistent with the observation that  $f(N) = \tau_u/N^{1+2\nu}$  is a monotonically decreasing function of  $N$ , as shown in Table III.

$N$	$\tau_u$	$\gamma(N) = \tau_u/N^{1+2\nu}$
16	$(3.53 \pm 0.06) \times 10^4$	$34.5 \pm 0.6$
24	$(1.01 \pm 0.02) \times 10^5$	$35.6 \pm 0.6$
32	$(2.04 \pm 0.04) \times 10^5$	$35.1 \pm 0.6$
46	$(4.96 \pm 0.09) \times 10^5$	$34.6 \pm 0.6$
64	$(1.10 \pm 0.02) \times 10^6$	$33.7 \pm 0.6$
90	$(2.56 \pm 0.04) \times 10^6$	$33.3 \pm 0.6$
128	$(6.1 \pm 0.1) \times 10^6$	$33.2 \pm 0.6$
180	$(1.44 \pm 0.02) \times 10^7$	$33.1 \pm 0.6$
256	$(3.38 \pm 0.06) \times 10^7$	$32.2 \pm 0.6$
500	$(1.73 \pm 0.03) \times 10^8$	$31.0 \pm 0.6$
1000	$(8.79 \pm 0.01) \times 10^8$	$27.9 \pm 0.4$

TABLE III. Mean unthreading time over 2,048 runs for each value of  $N$ .

## V. POLYMER'S MEMORY EFFECTS: THE THEORY OF TRANSLOCATION AND THE BFM

In Refs. [8, 9] we presented the theory of translocation, based on the polymer's memory effects. We now demonstrate that once these finite-size effects are taken into account, the polymer's memory effects for the BFM are consistent with that theory.

The theory we presented in Refs. [8, 9] is as follows. Translocation takes place via the exchange of monomers through the pore. This exchange responds to  $\phi(t)$ , the difference in chain tension perpendicular to the membrane; simultaneously,  $\phi(t)$  adjusts to  $v(t) = \dot{s}(t)$ , the transport velocity of monomers across the pore, as well. In the presence of memory effects,  $\phi(t)$  and  $v(t)$  are related to each other by  $\phi(t) = \int_0^t dt' \mu(t-t') v(t')$  via the memory kernel  $\mu(t)$ . This relation can be inverted to obtain  $v(t) = \int_0^t dt' a(t-t') \phi(t')$ . The uniqueness of the relation between  $\phi(t)$  and  $v(t)$  implies that in the Laplace transform language,  $\mu(k) = a^{-1}(k)$ , where  $k$  is the Laplace variable representing inverse time. Additionally, via the fluctuation-dissipation theorem,  $\mu(t-t')$  and  $a(t-t')$  are expressed as

$$\mu(t-t') = \langle \phi(t) \phi(t') \rangle_{v=0}; \quad a(t-t') = \langle v(t) v(t') \rangle_{\phi=0}. \quad (3)$$

In Refs. [8, 9] we showed that the polymer's memory kernel is given by  $\mu(t) \sim t^{-\frac{1+\nu}{1+2\nu}} \exp(-t/\tau_R)$ , in which  $\tau_R$  is the Rouse time; this result, together with Eq. (3) yields  $\tau_d \sim N^{2+\nu}$ . The derivation for the exponent  $(1+\nu)/(1+2\nu)$  of the power-law relies on three scaling relations for an equilibrated polymer of length  $n$  with one end tethered to a membrane: (i) the real-space distance between the free and the tethered end scales as  $n^\nu$ , (ii) its entropic spring constant scales as  $n^{-2\nu}$ , and (iii) its longest correlation time scales as  $n^{1+2\nu}$ . For the BFM, (i) holds for  $n$  not so large, but since the scalings (ii) and (iii) suffer from severe finite-size effects (as reported in Secs. III A and III B), we expect the  $t^{-\frac{1+\nu}{1+2\nu}}$  behavior of the power-law in  $\mu(t)$  to only manifest itself at long times. Note that “long times” here refers to times long compared to unity, but short in comparison to the longest relaxation time of the polymer; this implies that  $\mu(t) \sim t^{-\frac{1+\nu}{1+2\nu}}$  can only be observed when the polymer is long. Indeed, we demonstrate this below in Fig. 4, by measuring  $\mu(t-t') = \langle \phi(t) \phi(t') \rangle_{v=0}$  for the BFM for a polymer with length  $N = 1000$ , where we used the perpendicular-to-the-membrane distance  $Z_4$  of the center-of-mass of the first four monomers (counting from the pore) as a proxy for the chain tension [21]. More precisely,

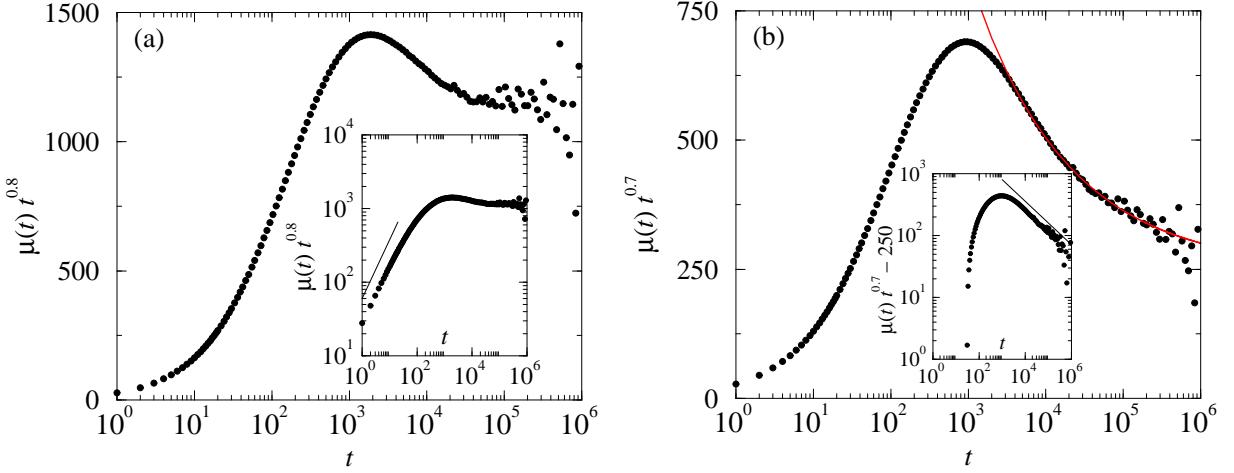


FIG. 4. The memory kernel  $\mu(t)$  for a polymer with length  $N = 1000$  for the BFM. (a) Demonstrates the lack of a single power-law  $\sim t^{-0.8}$ , (main graph: semi-log, inset: same data shown in log-log). The initial increasing part is caused by  $\mu(t)$  remaining practically constant till  $t \approx 500$ , this is shown by the solid line in the inset corresponding to an exponent 0.8. (b) However, given that we expect a behavior  $\mu(t) \sim t^{-(1+\nu)/(1+2\nu)} = t^{-0.7}$  [8, 9] for the BFM in 2D, we show that the late-time data can be numerically well-fitted by  $6400t^{-1.05} + 250t^{-0.7}$ , as shown by the red line. The inset demonstrates the existence of a second power-law behavior of  $\mu(t)$  at intermediate times: the solid line corresponds to the scaling  $\sim t^{-0.35}$ .

we tether the middle monomer of the polymer in the pore (this corresponds to  $v = 0$ ), and obtain good statistics for  $\langle \phi(t)\phi(t') \rangle$  over a total simulation time of  $4 \cdot 10^{10}$  attempted moves per monomer. As can be seen in Fig. 4(a),  $\mu(t) = \langle \phi(t)\phi(0) \rangle_{v=0}$  does not show a memory exponent 0.8. Moreover, given that we expect a behavior  $\mu(t) \sim t^{-(1+\nu)/(1+2\nu)} = t^{-0.7}$  [8, 9] for the BFM in 2D, Fig. 4(b) shows that  $\mu(t)$  can be fitted with a combination of power-laws  $\sim t^{-0.7}$  and  $\sim t^{-1.05}$  (see figure caption for details). The fact that the data can be fitted with this combination of power-laws does not constitute compelling evidence for  $\mu(t) \sim t^{-0.7}$ ; other exponents within a range of  $\pm 0.1$  can be fitted as well, with suitably chosen power-law corrections. The main point is, however, that our theoretically expected behavior  $\mu(t) \sim t^{-0.7}$  cannot be ruled out from these numerical data.

## VI. ANOMALOUS MONOMERIC MOBILITY FOR THE BFM IN AND NEAR THE PORE

So far we have discussed the finite-size effects in several basic equilibrium quantities for the BFM, and that the polymer's memory effects in the BFM do not rule out our theory of translocation that originally yielded  $\tau_d \sim N^{2+\nu}$  by relating the polymer's anomalous dynamics to its memory kernel; yet the asymptotic scaling behavior of  $\tau_d$  with  $N$  for the BFM is unknown at present. (It is the severity of the finite-size effects that makes scaling conclusions in relation to unbiased translocation for  $N \leq 256$  particularly meaningless). The answer to this conundrum lies in the dynamical peculiarity of the BFM, in particular how the BFM behaves dynamically (i.e., when  $v(t) = \dot{s}(t) = 0$ ) to the introduction of an obstacle, which, in the case at hand is the membrane with a narrow pore. To this end, we sample many polymer states (drawn from the equilibrium distribution), in which the polymer is tethered halfway through the pore with a width of two lattice spacings. For each of these states, for each monomer, we determine the individual monomeric mobilities. Since the orientation of the membrane breaks rotational symmetry, we separately keep track of the moves parallel and perpendicular to the membrane. The mobility of a monomer, parallel or perpendicular to the membrane, is defined by the acceptance probability of the corresponding MC move.

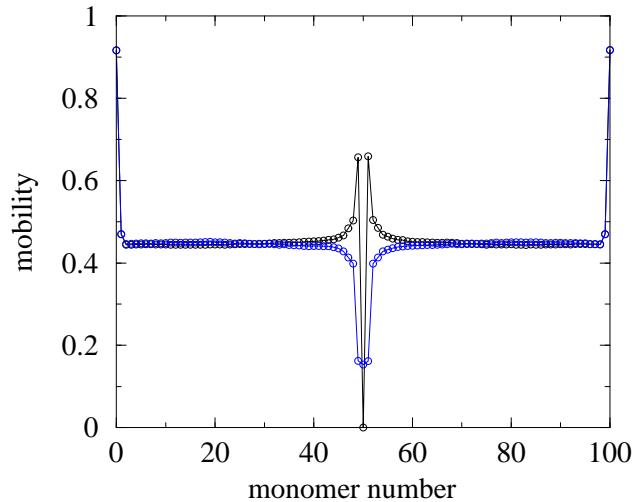


FIG. 5. Individual monomeric mobilities of a threaded polymer of length  $N = 100$  as a function of the monomer number. The polymer is tethered halfway through the pore, i.e., monomer number 50 is tethered in the pore. The mobility of each monomer is separately presented in terms of the moves parallel (blue) or perpendicular (black) to the membrane.

The individual monomeric mobilities for the BFM are shown in Fig. 5, for  $N = 100$  (with the 50th monomer tethered in the pore). On the one hand, the monomer located in the pore shows no mobility in the direction parallel to the membrane; this is to be expected, since sideways mobility of this monomer is forbidden due to the steric hindrance of the membrane. However, immediately outside the pore, the mobility of the monomers parallel to the membrane is strongly enhanced before it settles to a value  $\approx 0.44$  further away from the pore. On the other hand, the perpendicular-to-the-membrane mobilities of the threaded monomer and a few (two or three) of its nearest monomers are strongly hindered. Such anomalous behavior of the near-the-pore mobilities arises in the BFM since the presence of the membrane results in the stretching of the polymer around the pore, introducing an enhanced likelihood of maximally stretched bonds, which reduce the perpendicular-to-the-membrane mobilities of the threaded monomer and a few of its nearest monomers. The tendency of frozen mobility perpendicular to the membrane is peculiar for the specific types of moves allowed in the BFM (we have also checked that this continues to hold for longer polymers in the BFM, data not shown here). For instance, we verified that if a collective move of two neighboring monomers in the same direction is added to the dynamics, this tendency of frozen mobility is removed to a large extent. Note that in other models, as well as in experiment, reduced mobility (“friction”) in the pore can have various natural causes; although this can postpone the onset of scaling, it is not expected to change scaling exponents in the thermodynamic (long-chain) limit. It is noteworthy to mention here that in our lattice polymer model, in the neighborhood of the pore, the monomeric mobilities parallel to the membrane are reduced, while the perpendicular-to-the-membrane mobilities are marginally enhanced (not shown here).

From a theoretical point of view, in the limit of long polymers, either enhanced or reduced dynamics in the near vicinity of the pore — especially if there are only two or three monomers around the pore that suffer from anomalous mobility problems (as in Fig. 5) — should not change scaling exponents. However, such a statement is clearly not true for the BFM, as we demonstrate below that by enhancing the monomeric mobilities within a radius of 5 lattice sites around the pore (roughly twice the average bond length), one can significantly change the apparent exponent  $\alpha$ , towards our predicted theoretical value  $(1 + \nu)/(1 + 2\nu) = 0.7$ . It is indeed remarkable that enhancing the mobilities of typically two or three monomers around the pore changes the apparent exponent  $\alpha$  significantly for the BFM, even for fairly

long polymers.

### A. A modified BFM with enhanced monomeric mobilities around the pore

To investigate how much the anomalous mobility of the monomers around the pore in the BFM influences the dynamics of translocation, we perform simulations of the BFM in which all moves within a radius of 5 lattice sites around the pore are boosted by a (more or less arbitrary) factor 4. More precisely, all moves for all monomers located within a distance of 5 lattice sites from the pore, either before or after the move, are attempted four times more often than the other moves. Note that this does not violate detailed balance: for every move that is oversampled, the reverse move is also oversampled. The choice for these values in this modified BFM are both motivated by the data of Fig. 5; i.e., (i) in the original BFM model, typically only two or three monomers around the monomer that resides in the pore at any time suffer from reduced mobility and (ii) the factor of 4 is certainly enough to overcome even the reduced mobility of the monomer in the pore in the perpendicular-to-the-membrane direction, which for  $N = 100$  is approximately a factor 2.5 smaller than that of the monomer far away from the pore, and increases only slightly with polymer length. The unit of time in this modified model is still defined by one attempted MC moves per monomer far away from the membrane.

Figure 6 shows the anomalous dynamics of translocation — analogous to Fig. 3 — in this modified BFM: as can be seen therein, the apparent exponent  $\alpha$  has significantly decreased (from 0.84 in Fig. 3 to 0.765 in Fig. 6), towards the theoretical prediction  $(1 + \nu)/(1 + 2\nu) = 0.7$ . The corresponding apparent exponent  $\beta \approx 2.6$  up to  $N = 380$  (data not shown), larger than  $1 + 2\nu = 2.5$ , but smaller than  $2 + \nu = 2.75$ .

Additionally, for this modified BFM, we confirm that the memory kernel  $\mu(t - t') = \langle \phi(t)\phi(t') \rangle_{v=0}$  exhibits  $t^{-\frac{1+\nu}{1+2\nu}}$  behaviour as well. This is shown in Fig. 7 for a polymer with length  $N = 1000$ , where we also compare the data of Fig. 4. As can be seen in Fig. 7, the onset of the  $t^{-\frac{1+\nu}{1+2\nu}} = t^{-0.7}$  takes place at  $t \approx 1000$  for both models.

Note that the modification we made for mobilities of the monomers in the modified BFM is by no means what we can claim to be an exact compensation for the around-the-pore anomalous monomeric mobilities in the BFM, as seen in Fig. 5. Rather, the introduction of this modified model should be seen as an attempt to understand whether such anomalous

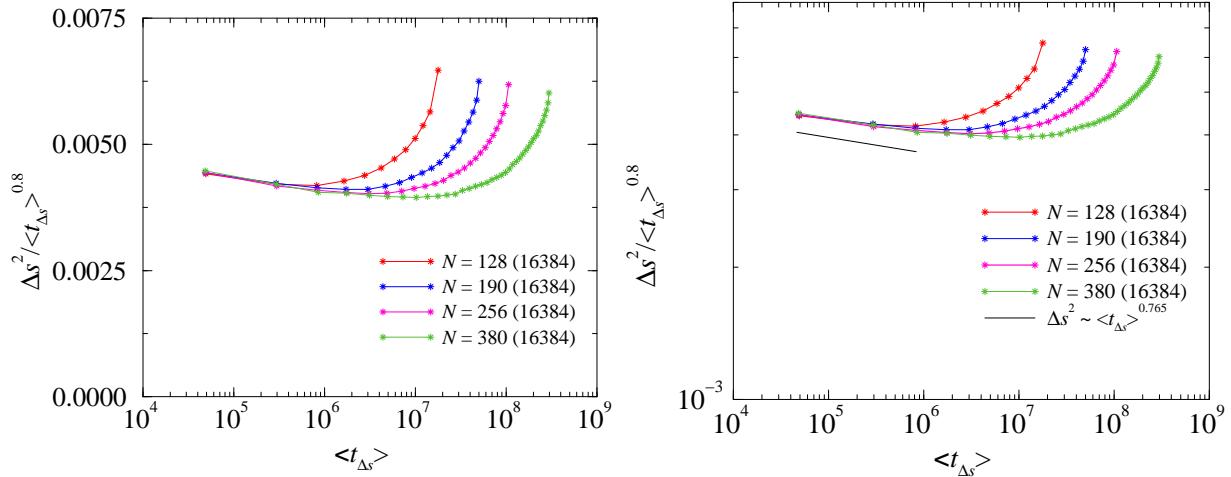


FIG. 6. Plots of  $\Delta s^2/\langle t_{\Delta s} \rangle^{0.8}$  as a function of  $\langle t_{\Delta s} \rangle$  with  $|\Delta s| = 5, 10, 15, \dots, N/2$ : semi-log (left panel), log-log (right panel), analogous to Fig. 3. The numbers in the parentheses in the legends denote the number of independent realizations over which the averages have been calculated. The lowest exponent  $\alpha$  for  $\langle \Delta s^2(t) \rangle \sim t^\alpha$  obtained for each curve is 0.765.

mobilities can account for the deviations from the expected values of  $\beta$ , namely  $2 + \nu = 2.75$ , albeit the polymer's memory effects in the BFM confirm our theory of translocation that originally yielded  $\tau_d \sim N^{2+\nu}$  by relating the polymer's anomalous dynamics to its memory kernel. The remarkable fact that for the BFM, enhancing the mobilities of typically two monomers around the pore changes the apparent exponent  $\alpha$ , even for fairly long polymers, combined with the fact that the memory kernel equals  $\mu(t-t') = \langle \phi(t)\phi(t') \rangle_{v=0} \sim (t-t')^{-\frac{1+\nu}{1+2\nu}}$  at long times, leads us to conclude that the anomalous mobilities of the monomers around the pore — peculiarities of the BFM — are indeed responsible for the deviations from our expected value of  $\beta$ , i.e.,  $2 + \nu$ . We thus conclude that the BFM is *not* a convenient model for cases where the polymer is constrained to pass through a narrow pore.

## VII. CONCLUSION AND OUTLOOK

In conclusion, in this paper we study unbiased polymer translocation in two-dimensions, with the Bond Fluctuation Model (BFM), in the absence of external forces on the polymer (i.e., unbiased translocation) and hydrodynamical interactions (i.e., the polymer is a Rouse polymer). While it has long been established that the pore-blockade time  $\tau_d$ , the characteristic time the polymer spends in the pore, asymptotically scales with the polymer length as

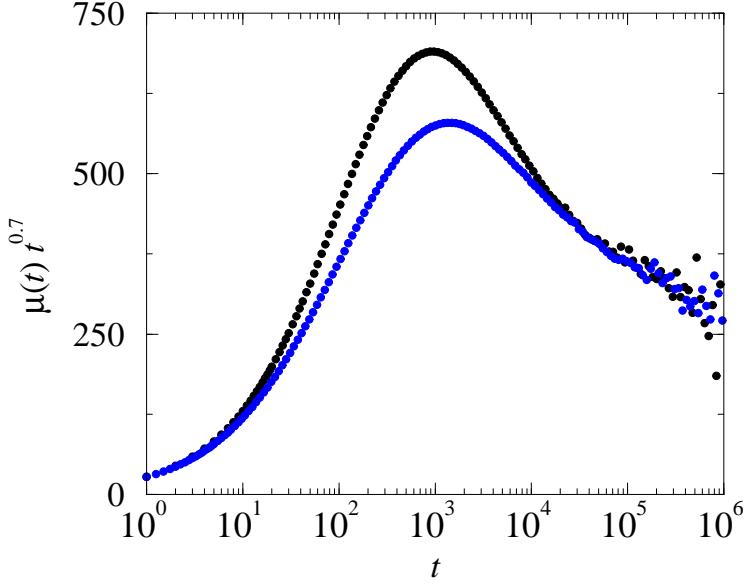


FIG. 7. The memory kernel  $\mu(t)$  for a polymer with length  $N = 1000$  for the BFM and the modified BFM. The data for the models are averaged over 80 and 560 independent realizations, over simulation times of  $5 \times 10^8$  and  $1.25 \times 10^8$  attempted moves per monomer per realization for the BFM and modified BFM, respectively.

$N^\beta$  for some  $\beta$ , earlier studies of unbiased polymer translocation, using the BFM, concluded that  $\beta = 1 + 2\nu$ , whereas a variety of other models produce results consistent with  $\beta = N^{2+\nu}$ , originally predicted by us. Here  $\nu$  is the Flory exponent of the polymer;  $\nu = 0.75$  in 2D. We find that for the BFM the quantity  $f(N) = \tau_d/N^{1+2\nu}$  is a monotonically decreasing quantity with increasing  $N$ , such that the rate of decrease for  $f(N)$  increases with increasing  $N$ . Having noted that with the BFM, the conclusion that  $\beta = 1 + 2\nu$  has been based on simulation data for  $N \leq 256$ , we further show in this paper that (i) the BFM suffers from strong finite-size effects for  $N \leq 256$ , and that (ii)  $f(N)$  decreases steeply for  $N > 256$ , the conclusion that  $\beta = 1 + 2\nu$  — in the usual sense of critical phenomena for polymers in the limit  $N \rightarrow \infty$  — is meaningless. We trace the peculiarities of the BFM to the anomalously low mobility of two or three monomers in the near vicinity of the pore, in the direction perpendicular to the membrane. We find that if the mobility of these monomers is enhanced, the exponent for the pore-blockade time increases towards  $2 + \nu$ . We conclude that, although the BFM is a fine model for polymer dynamics in general, it is not in situations where the polymer is constrained to pass through a narrow pore. Our analysis also implies that for those polymer models that assert  $\beta = 1 + 2\nu$ , one needs to thoroughly investigate their finite-size effects

and dynamical peculiarities, if such an assertion is to be proved meaningful.

A related issue regarding the use of the BFM for translocating polymers does still remain, and that is the case of field-driven translocation in two dimensions. For this situation, translocation is driven by a potential difference across the pore. (All results quoted below are for Rouse polymers.) First of all, using the same memory effects as in unbiased translocation, in Ref. [23] we argued that in 3D, the pore-blockade time exponent is  $(1+2\nu)/(1+\nu) \approx 1.37$ , and corroborated this result with extensive simulations; this result has now been verified with completely different polymer models [24, 25]. Further, in Ref. [10], we argued that for field-driven translocation in 2D, because of energy conservation, the pore-blockade time exponent has a lower bound  $2\nu = 1.5$ : for any field strength, a polymer length exists above which the Rouse friction prevents the transport of monomers from keeping up with the speed of translocation dictated by the memory effects. The exponent  $(1+2\nu)/(1+\nu)$  is therefore not observed for field-driven translocation in 2D. We also showed, numerically, using our lattice polymer model that in 2D the pore-blockade time exponent indeed turns out to be the same as its lower bound  $2\nu$  [10], which is in agreement with those obtained by the use of the BFM by two separate research groups [26, 27], who used  $N$  up to 600 and 256 respectively. However, a third group which also used the BFM claimed the pore-blockade time exponent for field-driven translocation in 2D to be consistent with  $2\nu$  for  $N$  up to 300, and  $1+\nu$  for  $N > 300$  [6, 28], which is clearly at odds with the results of Refs. [10, 26, 27]. If indeed the BFM finds the pore-blockade time exponent to be  $1+\nu$ , then the anomalous mobilities of the monomers around the pore, together with the finite-size effects, may explain why the exponent  $2\nu = 1.5$  is not observed in the BFM for field-driven translocation in two dimensions.

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[21] Since chain tension is not a directly measurable observable in the BFM, we considered the perpendicular-to-the-membrane distance  $Z_m$  of the center-of-mass of the first  $m$  monomers as a proxy for the chain tension [see for example Ref. [22], where we used  $m = 4$ ]. To verify that the local extension is indeed proportional to the chain tension at the pore, we performed separate simulations (not reported), in which we pulled on the free end of a tethered chain with a known (small) force  $f$ , and recorded  $\langle Z_m \rangle$ . It turned out that for  $m = 1$  or  $2$ ,  $\langle Z_m \rangle$  shows slightly non-linear behavior as a function of  $f$  for small forces, while for  $m = 4$  or higher,  $\langle Z_m \rangle$  is linear in  $f$  for small and medium-strength forces.

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